Ethyl hydroperoxide 3031-74-1 | DTXSID70184402

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Model	Data	

Weighted KNN model

5-fold CV (5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE	
0.87	0.81	0.87	0.82	0.86	0.86	

Model Results

Predicted value: 12.8 mol/L

Global applicability domain: Inside

Local applicability domain index: 4.77e-01

Confidence level: 9.17e-01

Nearest Neighbors from the Training Set

Image not found

Peracetic acid Measured: 13.1 Predicted: 11.7 Image not found

2-Methoxyethanol Measured: 13.1 Predicted: 13.2 Image not found

N-Methylethanolamine Measured: 13.3 Predicted: 13.0

Image not found

Glycidol Measured: 13.5 Predicted: 13.6 Image not found

2-Ethoxyethanol Measured: 11.1 Predicted: 11.1